Inherent Spin-Density-Wave Instability in Heavy-Fermion Superconductivity

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(Received 6 November 1986)

Both anisotropic superconducting (SC) states of heavy electrons with odd-parity p pairing and with even-parity d pairing are shown to have an inherent instability towards the spin-density wave which generally coexists with the SC state. A model is presented which contains an on-site repulsion characteristic of heavy-fermion materials, in addition to an intersite attraction. The second transition below the SC transition observed in $(U_{1-x}Th_x)Be_{13}$ is interpreted in terms of the spin-density-wave instability.

PACS numbers: 74.10.+f, 75.10.Lp, 75.30.Ds

Much attention has been focused on the so-called heavy-fermion systems recently.[1] It is now widely accepted that an unconventional superconductivity develops at low temperatures in some of these materials (UBe_{13}, UPt_3, and $CeCu_2Si_2$); namely, the superconducting (SC) gap vanishes at isolated lines or possibly at points on the Fermi surface (FS), although it is still highly controversial whether the SC state has odd parity or even parity. In this connection Th-doping experiments,[2-7] $(U_{1-x}Th_x)Be_{13}$, are crucial to our uncovering the nature of the unconventional superconductivity. As x increases, the SC transition temperature T_C first rapidly drops and then ceases to decrease, remaining at a relatively constant value of $x=2$–4 at.%.[2] In that concentration region a second phase transition is observed as a sharp peak in the specific-heat[2] and ultrasound[3] measurements.

Concerning this second transition several authors[8-10] have attempted to explain it theoretically in terms of a transition between different phases of nontrivial anisotropic superconductivity belonging to a multidimensional irreducible representation. However, the proposal based on this by Joynt, Rice, and Ueda[10] was not supported by a recent ultrasound experiment.[7]

Here we propose an alternative explanation: We interpret it as the transition to a spin-density-wave (SDW) state out of an unconventional SC state, both of which coexist below this transition. Although Batlogg *et al.*[3] have already suggested such an interpretation, no one has seriously examined this possibility so far. Needless to say, in a conventional isotropic singlet SC, the second-order phase transition to the SDW out of the SC state is impossible because the SC gap opens over all of the FS.[11]

In this respect we mention similar experiments on $(U_{1-x}Th_x)Pt_3$,[12] $U(Pt_{1-x}Pd_x)_3$,[13] and URu_2Si_2.[14] In the former two systems the doping induces a SDW state by suppression of the SC state. In the last system the SDW appears at $T_N=17$ K, coexisting with the SC state below $T_C=0.8$ K. These experiments undoubtedly indicate a sharp competition and delicate balance among various ground states (the SC state, magnetism, and also the normal-Fermi-liquid state) in heavy-fermion materials.

Since a physical origin of the observed anisotropic unconventional SC state with a pointlike (or linelike) gapless region on the FS comes from the strong on-site repulsion that prevents isotropic-singlet-pairing formation, the model should contain the repulsive interaction in the $l=0$ channel of the partial-wave decomposition as an essential ingredient, in addition to the attractive interaction in the $l=1$ channel (p-pairing case) or $l=2$ channel (d-pairing case). A possible microscopic origin of these interactions is discussed by Miyake *et al.*[15] and Ohkawa and Fukuyama.[16]

We shall demonstrate that nontrivial superconducting states with odd parity or even parity have an inherent instability towards the SDW by the very reason that the nontrivial SC state comes about. We shall study comparatively the p- and d-pairing cases and argue the experimental relevance of our results for $(U,Th)Be_{13}$.

We start with the following mean-field Hamiltonian (p-pairing case):

$$H=H_0+H_U+H_p, \qquad (1)$$

with

$$H_0=\sum_{k\sigma}\epsilon(k)C^\dagger_{k\sigma}C_{k\sigma},$$

$$H_U=\sum_k M(C^\dagger_{k+Q\uparrow}C_{k\downarrow}+\text{H.c.}),$$

$$H_p=-\sum_{k\sigma}[\Delta_p(k)C^\dagger_{k\sigma}C^\dagger_{-k\sigma}+\text{H.c.}],$$

where we assume the tight-binding model on a two-dimensional (2D) square lattice (the lattice constant $a\equiv1$), $\epsilon(k)=-t\gamma(k)=-t(\cos k_x+\cos k_y)$, and that the band is half filled to ensure the SDW nesting whose wave vector is $\mathbf{Q}=(\pi,\pi)$. The self-consistent conditions for the SDW and the SC order parameters, M and $\Delta_p(k)$, are given by

$$M=-U\sum_k\langle C^\dagger_{k+Q\uparrow}C_{k\downarrow}\rangle,$$

$$\Delta_p(k)=\sum_{k,\sigma}g_p(k,k')\langle C^\dagger_{k'\sigma}C^\dagger_{-k'\sigma}\rangle,$$

where U is the on-site Coulomb interaction. We assume a pairing interaction of the form $g_p(k,k')=g_p(\sin k_x\sin k_{x'}+\sin k_y\sin k_{y'})$ so that $\Delta_p(k)=\Delta_p\tau_p(k)$ is stabilized where $\tau_p(k)=(\sin k_x+i\sin k_y)/\sqrt{2}$. Thus this SC state has isolated points at which the gap vanishes on the 2D FS.

By diagonalizing (1), we obtain

$$\begin{aligned} 1 &= UT\textstyle\sum_{\omega_n}\sum_k \{\omega_n^2+\epsilon^2(k)+M^2-|\Delta_p(k)|^2\}/D(k,\omega_n),\\ 1 &= g_pT\textstyle\sum_{\omega_n}\sum_k |\tau_p(k)|^2\{\omega_n^2+\epsilon^2(k)-M^2+|\Delta_p(k)|^2\}/D(k,\omega_n),\\ D(k,\omega_n) &= [\omega_n^2+\epsilon^2(k)+|\Delta_p(k)+M|^2][\omega_n^2+\epsilon^2(k)+|\Delta_p(k)-M|^2]. \end{aligned} \tag{2}$$

Note that when $M\to 0$ and $\Delta_p\to 0$ the BCS-like equations are recovered as expected. These coupled equations completely determine M and Δ_p self-consistently.

Let us examine the SDW instability out of the p-pairing SC state via a second-order phase transition below T_C. (Thus the SDW and SC states generally coexist below T_N.) Taking $M\to 0$ and $T\to T_N$ in (2), we perform the 2D integrations over the first Brillouin zone in the reciprocal space of a square lattice by linearizing $\epsilon(k)$ about the FS ($t\gg T$). We obtain

$$\frac{1}{u}=2\pi T_N\sum_{|\omega_n|\le E_B}\left[\frac{1}{|\omega_n|}\ln\frac{2\pi t}{(\omega_n^2+\Delta_p^2)^{1/2}}-\frac{\Delta_p^2}{|\omega_n|(\omega_n^2+\Delta_p^2)}\right],\quad \frac{1}{\tilde g_p}=2\pi T_N\sum_{|\omega_n|\le E_C}\frac{1}{\Delta_p}\left[\frac{\pi}{2}-\tan^{-1}\frac{|\omega_n|}{\Delta_p}\right], \tag{3}$$

where $u=U/2\pi^2t$ and $\tilde g_p=2g_p/\pi^2t$ under the condition $T_N/\Delta_p>O(\Delta_p/t)$. The two energy cutoff parameters E_B and E_C are introduced. It is seen that it is *always* possible for the SDW to appear below T_C irrespective of U. {Note that there is an upper limit $u_{cr}\simeq[\ln(2e^\gamma E_B/\pi T_C)\ln(2t/\pi T_C)]^{-1}$, with γ the Euler constant, beyond which T_N becomes higher than T_C.} We point out, however, that T_N rapidly decreases as Δ_p increases since very few electrons remain available in the neighborhood of the gapless region on the FS for the formation of the SDW to work. We show the variation of T_N as a function of u in Fig. 1.

Let us now turn to the even-parity pairing case. We consider here a d pairing described by $\Delta_d(k)=\Delta_d\tau_d(k)$ with $\tau_d(k)=(\cos k_x-\cos k_y)/2$, assuming a pairing interaction of the form $g_d(k,k')=g_d\tau_d(k)\tau_d(k')$. The mean-field Hamiltonian corresponding to (1) is diagonalized to yield the coupled self-consistent equations

$$\begin{aligned} 1 &= UT\textstyle\sum_{\omega_n}\sum_k[\omega_n^2+\epsilon^2(k)+M^2+\Delta_d^2(k)]^{-1},\\ 1 &= g_dT\textstyle\sum_{\omega_n}\sum_k\tau_d^2(k)[\omega_n^2+\epsilon^2(k)+M^2+\Delta_d^2(k)]^{-1}. \end{aligned} \tag{4}$$

The structure of these equations is quite different from that of (2) for the p-pairing case, reflecting the symmetry of each SC order parameter. With the same approximation that leads to (3) ($t\gg T,\Delta_d$), we obtain by taking $M\to 0$ and $T\to T_N$

$$\frac{1}{u}=2\pi T_N\sum_{|\omega_n|\le E_B}\frac{\ln(2\pi t/|\omega_n|)}{(\omega_n^2+\Delta_d^2)^{1/2}},\quad \frac{1}{\tilde g_d}=2\pi T_N\sum_{|\omega_n|\le E_C}\left[\frac{\ln(2\pi t/|\omega_n|)}{(\omega_n^2+\Delta_d^2)^{1/2}}-\frac{1}{2\Delta_d}\ln\left(\frac{(\omega_n^2+\Delta d^2)^{1/2}+\Delta_d}{(\omega_n^2+\Delta d^2)^{1/2}-\Delta_d}\right)\right], \tag{5}$$

where $\tilde g_d=2g_d/\pi^2t$. It is easily seen that again the SDW *always* appears, irrespective of the value of U, via a second-order transition, although T_N is generally depressed by the presence of the d-pairing SC state as illustrated in Fig. 1.

From (3) and (5) near T_C and the SDW transition temperature T_{N0} without the SC state, we obtain the initial depression of T_N approximately ($t\gg T_{N0}$) as

$$(T_{N0}-T_N)/T_{N0}\simeq\begin{cases}(\Delta_p/2\pi T_{N0})^2\frac{21}{2}\zeta(3)[\ln(t/T_{N0})]^{-1}, & p\text{ pairing},\\ (\Delta_d/2\pi T_{N0})^2\frac{7}{2}\zeta(3), & d\text{ pairing},\end{cases}$$

where $\zeta(3)$ is the zeta function, implying that the initial depression in the d-pairing case is larger than that in the p-pairing case. The numerical calculations are shown in Fig. 2. In the present work even-parity d-pairing is very effective in preventing the formation of the SDW compared to the present odd-parity p pairing.

Since we have chosen the p- and d-pairing states such that on the 2D FS with square symmetry the gap vanishes at the points $\mathbf{k}=(\pi,0)$ (p case) or $\mathbf{k}=(\pi/2,\pi/2)$ (d case), the electrons in the ungapped region of the FS feel a residual repulsive interaction which ultimately leads the system to the SDW transition.[17] However, if the hypothetical SDW transition temperature T_{N0} in the absence of the SC state is much lower than T_C, the present d pairing virtually does not exhibit the SDW instability because T_N is heavily suppressed as shown in Fig. 2.

Here we should point out two experimental facts[2] relevant to our results: (1) In $(U_{1-x}Th_x)Be_{13}$ for $x=2-4$ at.% the second transition temperature takes its

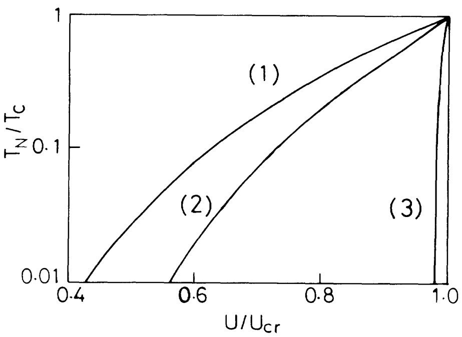

FIG. 1. Variation of the SDW transition temperature, normalized by T_N at $U=U_{cr}$, as a function of the on-site repulsion U/U_{cr}: curve 1, without the SC state; curve 2, in the presence of p pairing; and curve 3, in the presence of d pairing. ($E_B/T_C=500$, $E_C/T_C=300$, $t/T_C=1000$.)

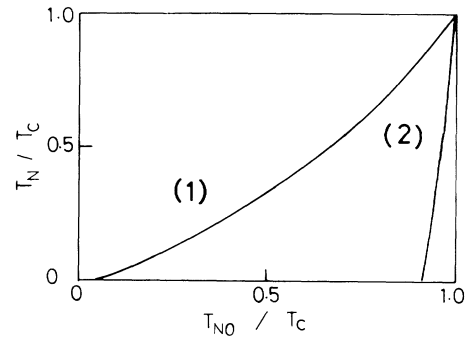

FIG. 2. Change of T_N in the p pairing (curve 1) and d pairing (curve 2) cases as a function of T_{N0}/T_C. ($E_B/T_C=500$, $E_C/T_C=500$, $E_C/T_C=300$, $t/T_C=1000$, $\tilde{g}_p=0.0652$, and $\tilde{g}_d=0.0446$.)

minimum when T_C exhibits a local maximum as a function of x [see Fig. 2(b) in Ref. 6]. (2) For $x \leq 2$ at.% the second transition does not appear at all when T_C is relatively high. Under the assumption that the dilute doping affects mainly T_C, these correlations between the two transition points T_C and T_N are qualitatively understandable if we identify the second transition as the SDW one: As shown before, T_N is a sensitively decreasing function of T_C for both the p- and d-pairing cases.

The NMR and muon-resonance experiments[5] show that the spontaneous sublattice moment is less than $\sim(10^{-2}\text{-}10^{-3})\mu_B/U$ if anything. This fact does not contradict our interpretation because in the present SDW state the electrons available to participate in the SDW formation are limited to only those in the ungapped region and its neighbor on the FS. Thus the spontaneous moment per U atom must be very small.

In conclusion, we have found an inherent SDW instability in the nontrivial anisotropic superconducting states. This comes from the very fact that the heavy-fermion systems are characterized by having an extremely narrow band on the FS and thus a strong repulsive interaction between quasiparticles with large effective mass.

We thank T. Ohmi, M. Fujita, and T. Tsuneto for useful discussions.

Note added.—We have further examined[18] the relative stability between the SDW and the various SC states. It turns out from symmetry considerations that to classify fully the SC states relative to the SDW, the parity symmetry (odd or even) and the translational symmetry (odd or even) by the nesting vector Q of the order parameter $\Delta(k)$ are both important; the less-competitive SC states are the *EO* states (even parity and odd under the translation) and *OE* states rather than the *OO* or *EE* states. This does not contradict Miyake, Schmitt-Rink, and Varma[19] and Scalapino, Loh, and Hirsch,[20] who claim that the even-parity pairing is stabilized by antiferromagnetic spin fluctuations.

[1]P. A. Lee *et al.*, Comments Condens. Matter Phys. **12**, 99 (1986); Z. Fisk *et al.*, Nature **320**, 6057 (1986); K. Miyake, J. Magn. Magn. Mater. (to be published).

[2]H. R. Ott *et al.*, Phys. Rev. B **31**, 1651 (1985).

[3]B. Batlogg *et al.*, Phys. Rev. Lett. **55**, 1319 (1985).

[4]H. M. Mayer *et al.*, Z. Phys. B **64**, 299 (1986).

[5]R. H. Heffner *et al.*, Phys. Rev. Lett. **57**, 1255 (1986). Also see D. E. MacLaughlin *et al.*, Phys. Rev. **53**, 1833 (1984).

[6]S. E. Lambert *et al.*, Phys. Rev. Lett. **57**, 1619 (1986).

[7]B. Batlogg *et al.*, J. Magn. Magn. Mater. (to be published).

[8]G. E. Volovik and D. E. Khmel'nitskii, Pis'ma Zh. Eksp. Teor. Fiz. **40**, 469 (1984) [JETP Lett. **40**, 1299 (1984)].

[9]L. P. Gor'kov and P. A. Kalugin, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 208 (1985) [JETP Lett. **41**, 253 (1985)].

[10]R. Joynt, T. M. Rice, and K. Ueda, Phys. Rev. Lett. **56**, 1412 (1986).

[11]K. Machida, J. Phys. Soc. Jpn. **50**, 2195 (1981).

[12]A. P. Ramirez *et al.*, Phys. Rev. Lett. **57**, 1072 (1986).

[13]A. de Visser *et al.*, J. Magn. Magn. Mater. **54–57**, 375 (1986); R. Verhoef *et al.*, Physica (Amsterdam) **142B**, 11 (1986).

[14]T. T. M. Palstra *et al.*, Phys. Rev. Lett. **55**, 2727 (1985); M. B. Maple *et al.*, Phys. Rev. Lett. **56**, 185 (1986); W. Schlabitz *et al.*, Z. Phys. B **62**, 171 (1986); F. R. de Boer *et al.*, Physica (Amsterdam) **138B**, 1 (1986); U. Walter *et al.*, Phys. Rev. B **33**, 7875 (1986); T. Kohara *et al.*, Solid State Commun. **59**, 603 (1986).

[15]K. Miyake, T. Matsuura, H. Jichu, and Y. Nagaoka, Prog. Theor. Phys. **72**, 1063 (1984).

[16]F. J. Ohkawa and H. Fukuyama, J. Phys. Soc. Jpn. **53**, 4344 (1984).

[17]We have done a similar calculation for another p-pairing state (the polar state), $\Delta_p(k)=\Delta_p(\sin k_x+\sin k_y)$, in which the gap vanishes at lines, and have proved the appearance of the SDW instability in this case too.

[18]M. Kato and K. Machida, to be published.

[19]K. Miyake, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **34**, 6554 (1986).

[20]D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch, Phys. Rev. B **34**, 3190 (1986).